

**WORKSHOP**

**"EUROPEAN YOUTH ACADEMIC SPRING 2006"**

**Sofia, Bulgaria, 3 - 7 April 2006**



**BOOK OF ABSTRACTS**

# Organizers

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## Workshop "European Youth Academic Spring 2006"

Sofia, Bulgaria, 3<sup>rd</sup> - 7<sup>th</sup> April, 2006

### PROGRAM

**Monday, 3<sup>rd</sup> April** : Arrival and Get-together cocktail at **19:00h**

In Kedar Hotel, "Shipchenski Prohod" Blvd. 50, Sofia-1113

**Tuesday, 4<sup>th</sup> April**

8:30 -9:30 Registration

9:30 - 9:45 Opening

9:45 -10:30 Introductory Lecture by a representative of NSFB (National  
Science Foundation of Bulgaria)

10:30 -10:50 Coffee break

### *Structure, properties and application of metal complexes*

*Chairman: Anife Ahmedova*

**10:50 - 11:25** **Ivayla Pantcheva**, Mono- and di- arylboronato platinum(II)

complexes as intermediates in transmetalation of  
arylboronic acids to Pt(II)(Ph)(DPPE)

**11:25 - 11:50** **Albert Figuerola**, When molecules become frustrated...

**11:50 - 12:15** **Valentina Getova**, A binuclear complex of copper(II) with  
the antihypertensive drug Labetalol: synthesis and  
properties

12:15 – 12:40

**Vladimira Videva**, New Metal Complexes Of Phosphinoyl-  
And Phosphoamide - Modified *p-tert-Butyl*-  
Calix[4]arenes

12:40 – 14:00

Lunch

### *Hydrogen bonding I*

*Chairman: Momchil Dimitrov*

14:00 – 14:25

**Miglena Georgieva**, Hydrogen bond – Thermochemical  
approach to its existence

14:25 – 14:50

**Nadezhda Markova**, Theoretical investigations on  
tautomeric equilibria in organic molecules taking into  
account the specific solvent effects

14:50 – 15:15

**Lalka Daskalova**, Computational and IR studies on carbonyl  
compounds: isolated molecules, anionic species and  
hydrogen bonded complexes

15:15 – 15:40

Coffee break

### *Hydrogen bonding II*

*Chairman: Momchil Dimitrov*

15:40 – 16:05

**Nadia Dozova**, Vibrational spectra and structure of NO-H<sub>2</sub>O,  
NO-HDO and NO-D<sub>2</sub>O complexes. An IR matrix  
isolation and DFT study.

16:05 – 16:30

**Bruno Madebène**, Large-amplitude coupled vibrations in the  
hydrogen bonded systems HF-H<sub>2</sub>O and HF-H<sub>2</sub>S

## Wednesday, 5<sup>th</sup> April

### *Spectroscopy in theory and practice I: application in analytical and*

*environmental sciences*

*Chairman: Tihomir Todorov*

9:00 – 9:25

**Milica Arsenovic**, Microelements determination in water and  
mussels (*Mytilus Galloprovincialis*) in Montenegro  
South Adriatic sea

9:25 – 9:50

**Dubravka Maravic**, Photoacoustic detection of the  
organophosphates

9:50 – 10:15

**Stanislav Bozhanov**, Determination of trace analytes in  
Lavender oil

10:15 – 10:35

Coffee break

### *Catalysis and enzyme kinetics*

*Chairman: Maya Guncheva*

10:35 – 11:00

**Senka Muselinovic**, Chemoenzymatic epoxidation of  
Soybean oil

11:00 – 11:35

**Vasil Atanasov**, Role of metal ion on enzyme action of  
Phospholipase A<sub>2</sub> from Bulgarian viper snake (*Vipera  
ammodytes meridionalis*)

## Theoretical Investigations on Tautomeric Equilibria in Organic Molecules Taking Into Account the Specific Solvent Effects

Nadezhda Markova, Venelin Enchev, Iliana Timcheva,  
Silvia Angelova

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The tautomeric equilibria of 2-aminothiazolidine-4-on, 4-aminothiazolidine-2-on and 5-fluorouracil were studied in the gas phase and in water solution using post-Hartree-Fock ab initio quantum chemical calculations. The values of proton transfer barriers in the isolated, mono- and polyhydrated tautomers of studied compounds were calculated for two different mechanisms of tautomerisation. In the absence of water, the process of proton transfer should not occur. Addition of water molecules decreases the barrier making the process faster, as the participation of two water molecules in a proton transfer reaction is more favourable than the participation of only one water molecule. The solvent effects were considered by explicit inclusion of three (four) water molecules, which model a first hydration shell around the solute. To estimate the effect of the medium (water) on the relative stabilities of the tautomers of the studied compounds we applied the polarizable continuum model. The basis set and electron correlation effects on the energy barriers of tautomerization and the energy differences between tautomers were analyzed.

## NOTES